

DATASHEET

Cmpd101

Product overview

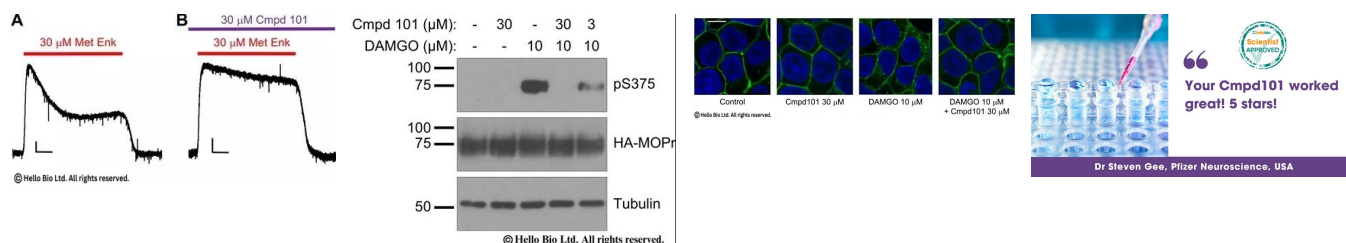
Name	Cmpd101
Cat No	HB2840
Alternative names	Compound 101; Takeda compound 101
Biological action	Inhibitor
Purity	>98%
Customer comments	<i>We would recommend Cmpd 101 from Hello Bio – it performs exactly as expected in assays looking at MOPr desensitisation, phosphorylation and internalisation. Dr Chris Bailey, University of Bath, UK and author on Mol Pharmacol paper, PubMed ID 26013542</i>

*Your **Cmpd101** – worked great! **Dr Steven Gee, Pfizer Neuroscience, USA***

*Your **Cmpd101** behaved as expected. **Verified customer, Monash University***

Description Novel, potent and selective GRK2/GRK3 inhibitor

Images



Biological Data

Biological description Cmpd101 (Compound 101) is a novel, potent and selective G-protein coupled receptor kinase 2 and 3 (GRK2/GRK3) inhibitor (IC_{50} values are 35 and 32 nM at GRK2 and GRK3 respectively).

Shows no activity at GRK5 at concentrations up to 125 μM and shows little activity at a broad range of other kinases.

Membrane permeable.

Cmpd101 can be used to study roles of GRK2/3 in GPCR desensitization and other functions.

Shown to potentiate phosphatidylinositol 4,5-bisphosphate (PIP₂) depletion and slow agonist-induced desensitization of protease-activated receptor 2 (PAR2).

Solubility & Handling

Storage instructions -20 °C

**Solubility overview
Handling**

Soluble in DMSO (100mM)

Hydroscopic solid, contact with air may cause material to become sticky. Product performance should not be affected but we recommend storing the material in a sealed jar.

Important

This product is for RESEARCH USE ONLY and is not intended for therapeutic or diagnostic use. Not for human or veterinary use.

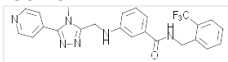
Chemical Data

Chemical name

3-[(4-methyl-5-pyridin-4-yl)-1,2,4-triazol-3-yl)methylamino]-N-[[2-(trifluoromethyl)phenyl]methyl]benzamide hydrochloride

Molecular Weight

502.92

Chemical structure**Molecular Formula**C₂₄H₂₁N₆OF₃.HCl**CAS Number**

865608-11-3

PubChem identifier

11677079

SMILES

CN1C(=NN=C1C2=CC=NC=C2)CNC3=CC=CC(=C3)C(=O)NCC4=CC=CC=C4C(F)(F)F

Source

Synthetic

InChi

InChI=1S/C24H21F3N6O/c1-33-21(31-32-22(33)16-9-11-28-12-10-16)15-29-19-7-4-6-17(13-19)23(34)30-14-18-5-2-3-8-20(18)24(25,26)27/h2-13,29H,14-15H2,1H3,(H,30,34)

InChiKey

WFOVEDJTASPCIR-UHFFFAOYSA-N

AppearanceYellow solid

References

Molecular mechanism of selectivity among G protein-coupled receptor kinase 2 inhibitors.

Thal et al (2011) Mol Pharmacol 80

PubMedID[21596927](#)**Role of G Protein-Coupled Receptor Kinases 2 and 3 in μ -Opioid Receptor Desensitization and Internalization.**

Lowe et al (2015) Mol Pharmacol 88(2)

PubMedID[26013542](#)**Contributions of protein kinases and β -arrestin to termination of protease-activated receptor 2 signaling.**

Jung et al (2016) J Gen Physiol 147(3)

PubMedID[26927499](#)**Distinct cortical and striatal actions of a β -arrestin-biased D2 receptor ligand reveal unique antipsychotic-like properties.**

Urs et al (2016) Proc Natl Acad Sci U S A 113(50)

PubMedID[27911814](#)**Agonist-selective recruitment of engineered protein probes and of GRK2 by opioid receptors in living cells**Stoeber et al (2019) bioRxiv <https://doi.org/10.1101/866780>
